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Development of a Model for a Continuous Ultra-Filtration System

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Due to the wide applicability and simplicity of the ultra-filtration process, it is currently being used in a variety of commercial processes for the purpose of separation and concentration of valuable products and/or recovery of raw materials from dilute systems [1]. A predictive model for a system derived from first principles, is instrumental in evading the costs of conducting time-consuming experiments while also allowing one to not be dependent on a trial and error analysis approach. The validated final model can serve to understand the operational issues of the process and from it identify the important phenomena occuring in the process and/or the corresponding model parameters. Also, it can help to design experiments to collect useful measured data.

Therefore, a model was systematically developed in four phases: define the system to be modelled; derive the model equations representing the system; analyze and numerically solve the model equations; calibrate, validate and apply the model for different studies [2]. The objectives for the model are that it should be able to predict the feed and retentate flow-rates along with the permeate flux from a continuous ultra-filtration (UF) system consisting of different geometry (and 'N' membrane stacks) used for the concentration of enzyme solutions from a known inlet concentration to a desired (target) outlet concentration during the recovery and/or downstream processing of enzymes. The envisaged purpose of this model is to improve the efficiency of the UF separation process. The final model, saved as a model object, should be possible to use for the specified objectives as well as model parameter sensitivity, importance of the involved phenomena (mass transfer, permeability, etc.). Also, the model object could be used in an external simulation environment to guide process operators to run the system under different operaional scenarios, such as operate at flow-rates specifically needed to take specified feed solutions to the desired outlet concentrations; or, to optimise the feed concentration to complete the process in a fixed time and many more. This could reduce the energy requirements when compared to running the process at the maximum pump flow-rate.

The developed steady-state model equations are organized in terms of conservation equations, constitutive equations and connection equations. Changing the process geometry changes the conservation and connection equations. Chaning the model assumptions and/or the chemical system or involved phenomena, changes the constitutive equations. Therefore, from a master generic model, different versions of problem specific models are generated and used for different model scenarios. For example, different candidate models for filtration through UF membranes, which could describe the possible phenomenon occurring during the UF process (for example concentration polarization, pore blocking, cake formation, adsorption on the membrane) [3] have been generated and their performance compared and evaluated by using different sets of constitutive equations in the model. The connection equations were formulated to relate the retentate and permeate concentrations by the retentivity of the membrane.

Among the different models studied, the perofrmance of a modified gel polarisation model was identified and was found to yield good results. Experimental data from the literature was used to estimate the parameters of the model, i.e., the mass transfer coefficients and an operational parameter, the gelling concentration, could be estimated for each enzyme using a least-squares fit of the objective function. The mass transfer coefficient from theoretical relations is known to be a function of diffusion coefficient, velocity of flow and the membrane spacer dimensions [4]. The diffusion coefficient, the most sensitive parameter of this model, was found to be a function of the feed concentration or the gelling concentration of the enzyme, depending on the operational scenario. This result also confirmed observations reported in published papers on this subject [5]. Considering that, the velocity of flow and the membrane spacer dimensions are almost constant throughout the system, the mass transfer coefficient was found to vary only with the feed concentration. Lastly, the model was validated against experimental data and can predict the flow-rates within a difference of +-20% of the experimental data.

The presentation will provide details of the developed model; the modelling tool used to develop, analyse and solve the model equations; estimation and sensitivity analysis of important model parameters; and the comparison and validation of the model bevahior with published data.

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